

FILE 'HOME' ENTERED AT 09:05:58 ON 22 AUG 2005

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 09:06:07 ON 22 AUG 2005

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STRUCTURE FILE UPDATES: 19 AUG 2005 HIGHEST RN 861198-35-8

DICTIONARY FILE UPDATES: 19 AUG 2005 HIGHEST RN 861198-35-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
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\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> s gsiishfrwgkpv/sqep

0 GSIISHFRWGKPV/SQEP

316548 SQL=13

L1 0 GSIISHFRWGKPV/SQEP

(GSIISHFRWGKPV/SQEP AND SQL=13)

=> s gsiishfrwgkp/sqep

0 GSIISHFRWGKP/SQEP

189979 SQL=12

L2 0 GSIISHFRWGKP/SQEP

(GSIISHFRWGKP/SQEP AND SQL=12)

=> s siishfrwgkp/sqep

0 SIISHFRWGKP/SQEP

84132 SQL=11

L3 0 SIISHFRWGKP/SQEP

(SIISHFRWGKP/SQEP AND SQL=11)

=> s s..sh.rwgkp/sqsp

L4 15 S..SH.RWGKP/SQSP

=> s l4 and sql<=11

668630 SQL<=11

L5 0 L4 AND SQL<=11

=> s .siishfrwgkpv/sqsp

L6 12 .SIISHFRWGKPV/SQSP

=> s 16 and sql=13  
316548 SQL=13

L7 10 L6 AND SQL=13

=> s caplus, uspatfull, uspat2  
0 CAPLUS  
0 USPATFULL  
0 USPAT2

L8 0 CAPLUS, USPATFULL, USPAT2  
(CAPLUS(W)USPATFULL(W)USPAT2)

=> s caplus, uspatfull, uspat2, biosis, scisearch, medline, embase  
0 CAPLUS  
0 USPATFULL  
0 USPAT2  
833 BIOSIS  
0 SCISEARCH  
0 MEDLINE  
0 EMBASE

L9 0 CAPLUS, USPATFULL, USPAT2, BIOSIS, SCISEARCH, MEDLINE, EMBASE  
(CAPLUS(W)USPATFULL(W)USPAT2(W)BIOSIS(W)SCISEARCH(W)MEDLINE(W)  
EMBASE)

=> fil caplus, uspatfull, uspat2, biosis, scisearch, medline, embase  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 132.90 133.11

FILE 'CAPLUS' ENTERED AT 09:09:16 ON 22 AUG 2005  
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CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 09:09:16 ON 22 AUG 2005  
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=> 17  
L7 IS NOT A RECOGNIZED COMMAND  
The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (=>).

=> s 17  
'13' NOT A VALID FIELD CODE  
'SQSP' IS NOT A VALID FIELD CODE  
L10 8 L7

=> dup remo 110  
PROCESSING COMPLETED FOR L10  
L11 8 DUP REMO L10 (0 DUPLICATES REMOVED)

=> d 111 1-8 bib abs

L11 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:345739 CAPLUS

DN 142:476398

TI Co-operative regulation of ligand binding to melanocortin receptor subtypes: evidence for interacting binding sites

AU Kopanchuk, Sergei; Veiksina, Santa; Petrovska, Ramona; Mutule, Ilze; Szardenings, Michael; Rinken, Ago; Wikberg, Jarl E. S.

CS Department of Pharmaceutical Biosciences, Uppsala University, Uppsala, 751 24, Swed.

SO European Journal of Pharmacology (2005), 512(2-3), 85-95

CODEN: EJPHAZ; ISSN: 0014-2999

PB Elsevier B.V.

DT Journal

LA English

AB This study evaluates the binding the MSH peptide analog [125I]NDP-MSH to melanocortin receptors MC1, MC3, MC4 and MC5 in insect cell membranes produced by baculovirus expression systems. The presence of Ca<sup>2+</sup> was found to be mandatory to achieve specific [125I]NDP-MSH binding to the melanocortin receptors. Although association kinetics of [125I]NDP-MSH followed the regularities of simple bimol. reactions, the dissociation of [125I]NDP-MSH from the melanocortin receptors was heterogeneous. Eleven linear and cyclic MSH peptides studied displaced the [125I]NDP-MSH binding to the studied melanocortin receptors, with the shapes of their competition curves varying from biphasic or shallow to super-steep (Hill coeffs. ranging from 0.4 to 1.5). Notably the same peptide often gave highly different patterns on different melanocortin receptor subtypes; e.g. the MC4 receptor selective antagonist HS 131 gave a Hill coefficient of 1.5 on the MC1 receptor but 0.5-0.7 on the MC3-5 receptors. Adding a mask of one of the peptides to block its high affinity binding did not prevent other competing peptides to yield biphasic competition curves. The data indicate that the binding of MSH peptides to melanocortin receptors are governed by a complex dynamic homotropic co-operative regulations.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:177849 CAPLUS

DN 139:1192

TI Redundancy of a functional melanocortin 1 receptor in the anti-inflammatory actions of melanocortin peptides: Studies in the recessive yellow (e/e) mouse suggest an important role for melanocortin 3 receptor

AU Getting, Stephen J.; Christian, Helen C.; Lam, Connie W.; Gavins, Felicity N. E.; Flower, Roderick J.; Schioeth, Helgi B.; Perretti, Mauro

CS The William Harvey Research Institute, London, UK

SO Journal of Immunology (2003), 170(6), 3323-3330

CODEN: JOIMA3; ISSN: 0022-1767

PB American Association of Immunologists

DT Journal

LA English

AB The issue of which melanocortin receptor (MC-R) is responsible for the anti-inflammatory effects of melanocortin peptides is still a matter of debate. Here the authors have addressed this aspect using a dual pharmacol. and genetic approach, taking advantage of the recent characterization of more selective agonists/antagonists at MC1 and MC3-R as well as of the existence of a naturally defective MC1-R mouse strain, the recessive yellow (e/e) mouse. RT-PCR and ultrastructural analyses showed the presence of MC3-R mRNA and protein in peritoneal macrophages (Mφ) collected from recessive yellow (e/e) mice and wild-type mice. This receptor was functional as Mφ incubation (30 min) with melanocortin peptides led to accumulation of cAMP, an effect abrogated by the MC3/4-R antagonist SHU9119, but not by the selective MC4-R antagonist HS024. In vitro Mφ activation, determined as release of the CXC chemokine KC and IL-1β, was inhibited by the more selective MC3-R agonist γ2-MSH but not by the selective MC1-R agonist MS05. Systemic treatment of mice with a panel of melanocortin peptides inhibited IL-1β release and PMN accumulation elicited by urate crystals in the

murine peritoneal cavity. MS05 failed to inhibit any of the inflammatory parameters either in wild-type or recessive yellow (e/e) mice. SHU9119 prevented the inhibitory actions of  $\gamma$ 2-MSH both in vitro and in vivo while HS024 was inactive in vivo. In conclusion, agonism at MC3-R expressed on peritoneal M $\phi$  leads to inhibition of exptl. nonimmune peritonitis in both wild-type and recessive yellow (e/e) mice.

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:575684 CAPLUS

DN 139:302161

TI Dissection of the anti-inflammatory effect of the core and C-terminal (KPV)  $\alpha$ -melanocyte-stimulating hormone peptides

AU Getting, Stephen J.; Schioeth, Helgi B.; Perretti, Mauro

CS The William Harvey Research Institute, London, UK

SO Journal of Pharmacology and Experimental Therapeutics (2003), 306(2), 631-637

CODEN: JPETAB; ISSN: 0022-3565

PB American Society for Pharmacology and Experimental Therapeutics

DT Journal

LA English

AB In this study, we analyzed the anti-inflammatory effects of  $\alpha$ -MSH (MSH)11-13 (KPV) in comparison with other MSH peptides in a model of crystal-induced peritonitis. Systemic treatment of mice with KPV,  $\alpha$ -MSH, the core melanocortin peptide His-Phe-Arg-Trp, and the melanocortin receptor 3/4 agonist Ac-Nle4-c[Asp5,D-Phe7,Lys10]NH<sub>2</sub> ACTH4-10 (MTII) but not the selective MC1-R agonist H-Ser-Ser-Ile-Ile-Ser-His-Phe-Arg-Trp-Gly-Lys-Pro-Val-NH<sub>2</sub> (MS05) resulted in a significant reduction in accumulation of polymorphonuclear leukocyte in the peritoneal cavity. The antimigratory effect of KPV was not blocked by the MC3/4-R antagonist Ac-Nle4-c[Asp5,D-2Nal7,Lys10]NH<sub>2</sub> ACTH4-10 (SHU9119). In vitro, macrophage activation, determined as release of KC and interleukin (IL)-1 $\beta$  was inhibited by  $\alpha$ -MSH and MTII but not by KPV. Furthermore, macrophage activation by MTII led to an increase in cAMP accumulation, which was attenuated by SHU9119, whereas KPV failed to increase cAMP. The anti-inflammatory properties of KPV were also evident in IL-1 $\beta$ -induced peritonitis inflammation and in mice with a nonfunctional MC1-R (recessive yellow e/e mice). In conclusion, these data highlight that the C-terminal MSH peptide KPV exhibits an anti-inflammatory effect that is clearly different from that of the core MSH peptides. KPV is unlikely to mediate its effects through melanocortin receptors but is more likely to act through inhibition of IL-1 $\beta$  functions.

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:380906 CAPLUS

DN 135:480

TI A process for identifying the active site in a biological target

IN Lundstedt, Torbjorn; Andersson, Per; Wikberg, Jarl; Muceniece, Ruta; Prusis, Peteris

PA Melacure Therapeutics AB, Swed.; Pett, Christopher Phineas

SO PCT Int. Appl., 101 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001036980	A2	20010525	WO 2000-GB4420	20001120
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,				

MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2001015305 A5 20010530 AU 2001-15305 20001120  
PRAI GB 1999-27346 A 19991118  
WO 2000-GB4420 W 20001120

AB Processes are provided for characterizing the sites of interaction between a Ligand Y and a Target X, comprising (1) inputting information on the chemical/phys. properties of at least two targets of the type X; (2) inputting information on the chemical/phys. properties of at least two ligands of the type Y; (3) inputting information on the interactions between at least two of the targets of type X with at least two of the ligands of type Y; and then correlating the information from steps 1, 2 and 3 using one or more multivariate methods in order to produce a model of the interaction between the Ligand Y and Target X, from which the sites of interaction may be identified and/or characterized. The processes of the invention are useful e.g. for drug design.

L11 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:44273 CAPLUS

DN 134:173140

TI PLS modeling of chimeric MS04/MSH-peptide and MC1/MC3-receptor interactions reveals a novel method for the analysis of ligand-receptor interactions

AU Prusis, P.; Muceniece, R.; Andersson, P.; Post, C.; Lundstedt, T.; Wikberg, J. E. S.

CS Department of Pharmaceutical Pharmacology, Uppsala University, Uppsala, SE-751 24, Swed.

SO Biochimica et Biophysica Acta (2001), 1544(1-2), 350-357

CODEN: BBACAQ; ISSN: 0006-3002

PB Elsevier Science B.V.

DT Journal

LA English

AB A novel method has been developed for the anal. of ligand-receptor interactions. The method utilizes binding data generated from the anal. of chimeric proteins with chimeric peptides. To each chimeric part of the peptide and receptor are assigned descriptors, thus creating a matrix of X descriptors. These descriptors are then correlated with the exptl. determined interaction binding affinities for each chimeric receptor/peptide pair by use of partial least-squares projection to latent structures (PLS). The method was applied to analyze the interactions of chimeric MSH-peptides with wild-type MC1 and MC3 receptors, and MC1/MC3 receptor chimeras (in total 40 peptide-receptor combinations). Two types of PLS models could be created, one that revealed the relationships between receptor and peptide structure and peptide binding pK<sub>i</sub> values (i.e., affinity) (R<sup>2</sup> and Q<sup>2</sup> being 0.71 and 0.62, resp.), and another that revealed the relationships between peptide and receptor structure and peptide-receptor selectivity (R<sup>2</sup> and Q<sup>2</sup> being 0.64 and 0.57, resp.). After addition of cross-terms these models improved significantly; the R<sup>2</sup> and Q<sup>2</sup> being 0.93 and 0.75 for affinity, and 0.92 and 0.72 for selectivity, resp. The anal. shows that the high affinity of the MSH-peptides is primarily achieved by interactions of the peptides' C-terminal amino acids with TM2 and TM3 of the receptor, and, to a lesser extent, by the interaction of the N-terminus with TM1, TM2 and TM3 of the receptor. However, in contrast, the MC1 receptor selectivity is primarily determined by an interaction of the peptides' N-termini with TM2/3 of the receptor. Moreover, the cross-terms of the PLS model revealed the existence of a strong interaction between TM6/7 and TM2/3 of the receptors.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:44265 CAPLUS

DN 134:173147

TI Detection of regions in the MC1 receptor of importance for the selectivity of the MC1 receptor super-selective MS04/MS05 peptides

AU Muceniece, R.; Mutule, I.; Mutulis, F.; Prusis, P.; Szardenings, M.;

Wikberg, J. E. S.  
CS Department of Pharmaceutical Pharmacology, Uppsala University, Uppsala,  
SE-751 24, Swed.  
SO Biochimica et Biophysica Acta (2001), 1544(1-2), 278-282  
CODEN: BBACAQ; ISSN: 0006-3002  
PB Elsevier Science B.V.  
DT Journal  
LA English  
AB The authors have investigated the ability of the authors' earlier  
identified MS04-MS05 MSH-peptide analogs to bind to chimeric MC1-MC3  
receptors. While the MS04 and MS05 peptides bind with nanomolar and  
sub-nanomolar affinities to the wild type MC1 receptor, they bind only  
with micromolar affinities for the wild type MC3 receptor, thus being the  
hitherto most MC1 receptor selective ligands. Upon exchanging portions  
involving transmembrane regions TM1, TM2-3, and TM6-7 of the MC1 receptor  
with corresponding portions of the MC3 receptor both of these peptides  
showed major losses of affinities. By contrast exchanges involving TM4-5  
did not appreciably affect the affinity of either MS04 or MS05. The  
authors' data suggest that the binding pocket for the MS04-MS05  
MSH-peptides is located between TM1-3 and TM6-7 of the melanocortin  
receptors.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 2000:237876 CAPLUS  
DN 133:12854  
TI New highly specific agonistic peptides for human melanocortin MC1 receptor  
AU Szardenings, M.; Muceniece, R.; Mutule, I.; Mutulis, F.; Wikberg, J. E. S.  
CS Department of Pharmaceutical Pharmacology, Uppsala University, Uppsala,  
SE-751 24, Swed.  
SO Peptides (New York) (2000), 21(2), 239-243  
CODEN: PPTDD5; ISSN: 0196-9781  
PB Elsevier Science Inc.  
DT Journal  
LA English  
AB A peptide with very high specificity for the human melanocortin MC1  
receptor identified by phage display was used as a lead for the design of  
new peptides. Two new peptides, MS05 and MS09, were synthesized and found  
to bind with sub-nanomolar affinities to the MC1 receptor. Both these  
peptides showed strong agonistic activity at the MC1 receptor. The MS05  
was the most MC1 receptor selective as it showed virtually no binding  
affinity for the MC4 and MC5 receptors and only micromolar affinity for  
the MC3 receptor. The selectivity and potency of the new peptides make  
them potent tools for studies of MC1 receptors, as well as novel potential  
candidate drugs for the treatment of inflammatory conditions.

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 1999:723063 CAPLUS  
DN 131:332097  
TI Melanotropin analogs as selective ligands for melanocortin 1 receptor and  
their use in the treatment of inflammation  
IN Szardenings, Michael; Muceniece, Ruta; Mutule, Ilze; Mutulis, Feliks;  
Wikberg, Jarl  
PA WA Pharm AB, Swed.  
SO PCT Int. Appl., 93 pp.  
CODEN: PIXXD2  
DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9957148	A1	19991111	WO 1999-GB1388	19990505
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, CZ, DE, DE, DK, DK, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,				

LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD,  
 SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU,  
 ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,  
 ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,  
 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2327550 AA 19991111 CA 1999-2327550 19990505  
 AU 9937222 A1 19991123 AU 1999-37222 19990505  
 AU 765120 B2 20030911  
 EP 1075492 A1 20010214 EP 1999-919433 19990505

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, FI

JP 2002513555 T2 20020514 JP 2000-547116 19990505  
 NZ 507792 A 20031031 NZ 1999-507792 19990505

PRAI SE 1998-1571 A 19980505  
 WO 1999-GB1388 W 19990505

OS MARPAT 131:332097

AB Substitution and side chain modification analogs of melanotropins that  
 show high selectivity and high affinity for MC1 receptors in combination  
 with effective stimulation or inhibition of cAMP formation in MC1  
 receptor-bearing cells, but low affinity for other subtypes of MC  
 receptors are described. These substances may be used to treat a wide  
 range of inflammatory conditions. Also disclosed is a DNA mol. and a  
 corresponding vector encoding the compound, a fusion protein comprising a  
 copy of it, a vector comprising DNA encoding the fusion protein, and a  
 pharmaceutical composition comprising the compound The peptide SSIISHFRWGKPV-NH2  
 (MS05) was synthesized by Fmoc chemical It had a Ki for the MC1 receptor of  
 0.76 nM, comparable to that of 0.68 nM for  $\alpha$ -MSH. The Ki of MS05  
 for MC3 was 1365 nM, compared to 52.3 for  $\alpha$ -MSH, and >>50,000 for  
 MC4 and MC5. MS05 was about as effective as  $\alpha$ -MSH in stimulating  
 cAMP formation in MC1-bearing cells.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 09:05:58 ON 22 AUG 2005)

FILE 'REGISTRY' ENTERED AT 09:06:07 ON 22 AUG 2005

L1 0 S GSIISHFRWGKPV/SQEP  
 L2 0 S GSIISHFRWGKP/SQEP  
 L3 0 S SIISHFRWGKP/SQEP  
 L4 15 S S..SH.RWGKP/SQSP  
 L5 0 S L4 AND SQL<=11  
 L6 12 S .SIISHFRWGKPV/SQSP  
 L7 10 S L6 AND SQL=13  
 L8 0 S CAPLUS, USPATFULL, USPAT2  
 L9 0 S CAPLUS, USPATFULL, USPAT2, BIOSIS, SCISEARCH, MEDLINE, EMBASE

FILE 'CAPLUS, USPATFULL, USPAT2, BIOSIS, SCISEARCH, MEDLINE, EMBASE'  
 ENTERED AT 09:09:16 ON 22 AUG 2005

L10 8 S L7  
 L11 8 DUP REMO L10 (0 DUPLICATES REMOVED)